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Tuned Range-Separated Density Functional Theory and Dyson Orbital Formalism for Photoelectron Spectra

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Abstract

© 2018 American Chemical Society. Photoelectron spectroscopy represents a valuable tool to analyze structural and dynamical changes in molecular systems. Comprehensive interpretation of experimental data requires, however, involvement of reliable theoretical modeling. In this work, we present a protocol based on the combination of well-established linear-response time-dependent density functional theory and Dyson orbital formalism for the accurate prediction of both ionization energies and intensities. Essential here is the utilization of the optimally tuned range-separated hybrid density functionals, improving the ionization potentials not only of frontier but also of the deeper lying orbitals. In general, the protocol provides accurate results as illustrated by comparison to experiments for several gas-phase molecules, belonging to different classes. Further, we analyze possible pitfalls of this approach and, namely, discuss the ambiguities in the choice of optimal range-separation parameters, the influence of the stability of the ground state, and the spin contamination issues as possible sources of inaccuracies.

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